IMPROVED MODELING APPROACH FOR HEAT SINK TOPOLOGY OPTIMIZATION

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ABSTRACT

The ongoing pursuit for higher power densities in electronic devices poses severe demands on cooling solutions. To explore the full potential of liquid-cooled microchannel heat sinks, topology optimization has been proposed as a method to optimize the microchannel layout. This has led to novel tree-like microchannel layouts. However, deficiencies in the porous medium models used thus far often lead to designs with disconnected channels, that cannot be used in practice. In this contribution, a new modeling approach is proposed for microchannel based heat sink topology optimization. A virtual pressure is introduced in the solid phase of the topology. This pressure field together with a zero velocity field in the solid then can be used for the regularization of the binary design variable. As a result, continuous optimization techniques can be used. This leads to improved results compared to optimization based on porous medium models for the solid phase. Indeed, in the latter case small leakage flows through the solid need to be tolerated in the numerical implementation, leading to inaccurate thermal modeling or ill-conditioned matrix systems. The approach presented in this paper circumvents these problems. The absence of penetration in our new model is demonstrated by two benchmarks. Performance of this model for optimization is validated by a hydraulic inverse design problem.

KEY WORDS: optimal control, topology optimization, Stokes equations, electronic equipment cooling, heat sinks

1. INTRODUCTION

Due to the increasing power densities in micro-electronics devices, more efficient cooling designs are required [9]. To explore the full potential of microchannel heat sinks, topology optimization has been proposed to determine the ideal distribution of microchannels through the heat sink. The philosophy is to formulate the design problem as a numerical optimization problem, where an optimal design is sought that minimizes an objective function subject to constraints. Typically, an artificial intermediate material with mixed liquid-solid properties is brought into the simulation. Material properties in each discretized cell are updated during the optimization procedure, pushing the artificial material towards either solid or fluid in the end. This has led to novel tree-like microchannel layouts with significantly enhanced performance [4].

Topology optimization in fluid problems is first introduced by Borrvall and Petersson [3], where a generalized Stokes equation with a Darcy type penalty term is used to model the flow in the artificial intermediate material. Next, topology optimization for channel flow problems is studied in Ref. [7]. Topology optimization of unsteady Navier-Stokes flow is performed in Ref. [6]. Others have applied topology optimization to thermal design. Convective heat transfer problems are studied in Refs. [1], [2], [5], [10], [11] and [12].

This work starts from earlier studies for liquid-cooled heat sinks under pressure-driven convection in Ref. [14,

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15], where Borrvall's model [3] is adopted. The problem with this model is that the velocity in the solid is never exactly zero, even with a very low permeability. As a result, there are always small, artificial leakage flows through the 'solid' phase.

In a hydraulic problem this is often not problematic, as the objective is usually to minimize the dissipated power. In such problems, the optimized design tends to avoid splitting big channels into smaller ones, since this would increase the viscous dissipation for a prescribed mass flow. The small leakage flows in the final designs do not affect the global performance of the design, leading to credible optimization results.

However, for cooling problems the situation is different. Now, the objective is typically to minimize the heat resistance for a given pressure drop. From a physical point of view, many fine channels are beneficial for the heat transfer towards the fluid. The optimizer tends to exploit the small but finite penetration velocity in solid, as the small leakage flows lead to very efficient convective cooling of the 'solid'. This leads to designs with a network of very fine channels which are often disconnected [14, 15]. However, the cooling of the solid phase due to the leakage flows is an artefact of the porous medium model and severely compromises the accuracy of the thermal model for the final solid-liquid design. This behavior can be somewhat mitigated by driving the inverse permeability of the solid towards infinity, but the resulting system quickly becomes ill-conditioned.

Guest and Prévost [8] have developed a different model to overcome the difficulty of no-slip condition. However, their model still cannot satisfy the no-penetration condition.

In this paper, we describe a new hydraulic model that can satisfy the no-penetration condition, thus providing a way to form the basis for reliable thermal heat sink optimization. This model and its implementation are introduced in section 2. In section 3, we present the results of some benchmark cases providing the absence of penetration through the solid. In section 4, we apply the new model to an inverse design problem. Finally, conclusions are drawn in Section 5.

2. MODEL EQUATIONS AND IMPLEMENTATION

To discuss the model equations conveniently, a schematic view of the heat sink is shown in Fig.1. It is a microchannel based heat sink. The top layer consists of both solid and fluid domains. That is the design space where we seek to find the optimal distribution of microchannels with improved cooling performance. The bottom layer is fixed solid and the heat source is a constant heat flux at the bottom of the heat sink.

In our model, we use the Stokes equations to simulate the fluid flow in the top layer. Since the flow in a heat sink for microchips (typical size of $10 \times 10 \text{ mm}^2$) is usually of the order of 10 m/s , typically the Re number is less than 0.1, so that the flow can be reasonably approximated by creeping flow. The governing equations in the fluid domain Ω_f are

$$\begin{cases} -\mu \nabla \cdot \nabla \vec{u} + \nabla p = 0, & \text{in } \Omega_f, \\ \nabla \cdot \vec{u} = 0, & \text{in } \Omega_f. \end{cases} \quad (1)$$

Fig. 1 Schematic layout of microchannel based heat sink [14].

In these equations, $\vec{u}$ is the velocity vector, p the pressure, and μ the viscosity of the fluid. This model for the fluid is complemented with zero-slip conditions at all boundaries and interfaces with the solid phase.

For purely solid-fluid designs, the velocity and the pressure in the solid phase do not impact the solution in the fluid phase. Hence, we are free to choose any model for the solid. To achieve the no-penetration condition in the solid, a solid model is constructed by imposing velocities equal to zero. This can be interpreted as a still fluid with an artificial body force being implicitly introduced to balance the pressure gradient in the Stokes equation, in such a way that the pressure in the solid can be assumed to be equal to the pressure in this still fluid. The control equations in the solid domain Ω_s can be written as

$$\begin{cases} \vec{u} = 0, & \text{in } \Omega_s, \\ \nabla \cdot \nabla p = 0, & \text{in } \Omega_s. \end{cases} \quad (2)$$

We remark that by construction the velocity field in the combined fluid-solid domain will be continuous at the solid-liquid interface. To ensure also continuity of the pressure field, we impose the requirement that the solid and liquid pressures should be equal at the interface as an interface condition for the Laplace equation in the solid. In the resulting model, the mass flux is conserved.

Using an interpolation of this model with the Stokes equations for the fluid, a design parameterization for continuous optimization is implemented. The momentum equation of the new model is

$$-\mu \nabla \cdot \nabla \vec{u} + \nabla p + c(\varepsilon) \vec{u} = 0, \quad \text{in } \Omega. \quad (3)$$

Zero velocity in the solid regions can be enforced without the problem becoming ill-conditioned. For intermediate, porous material, the resulting momentum equation resembles a Darcy-penalized Stokes model, where the interpolation coefficient $c(\varepsilon)$ becomes the inverse permeability introduced in Ref. [3]. The implementation of the continuity equation ensures the velocity field is divergence free for all values of the porosity, providing an automatic transition from fluid model to solid models. Design variable is ε , with the limits $\varepsilon = 0$ for solid and $\varepsilon = 1$ for fluid. The resulting model is equivalent to a Darcy-penalization with $c(\varepsilon) \rightarrow 0$ for $\varepsilon \rightarrow 1$ and $c(\varepsilon) \rightarrow \infty$ for $\varepsilon \rightarrow 0$.

The discretization of the model equations is performed on a uniform Cartesian grid with a finite volume method. To avoid checkerboard pressure distribution, a staggered grid is employed comparable to the approach in Ref. [16]. The pressure and design variables are positioned at cell-centers, while velocity components are distributed at cell faces. The discretized equations are solved with a coupled solver to solve for velocities and pressure simultaneously.

3. VALIDATION OF THE FORWARD SIMULATION

To validate our new model, we first apply it to simulate the flow in a few representative test cases in this section, before applying it to a topology optimization problem in section 4. Here, we assess the absence of penetration through the solid in our model and compare the results with those of existing porous medium models. We compare to both Borrvall's model [3],

$$\begin{cases} -\mu \nabla \cdot \nabla \vec{u} + \nabla p + \alpha(\varepsilon) \vec{u} = 0, & \text{in } \Omega, \\ \nabla \cdot \vec{u} = 0, & \text{in } \Omega, \end{cases} \quad (4)$$

and Guest's model [8],

$$\begin{cases} \varepsilon(-\mu \nabla \cdot \nabla \vec{u}) + \nabla p + (1 - \varepsilon) \frac{\mu}{k_s} \vec{u} = 0, & \text{in } \Omega, \\ \nabla \cdot \vec{u} = 0, & \text{in } \Omega. \end{cases} \quad (5)$$

Fig. 2 Layouts of forward validation benchmarks.

In these equations $\mu = 1.004 \times 10^{-3} Pa \cdot m$, and $\varepsilon(\mathbf{x}) = \frac{\text{volume of fluid}}{\text{volume of all}}$ is the design variable in a small neighbourhood around $\mathbf{x}$. In Borrvall's case, $\alpha(\varepsilon) = \alpha_s + (\alpha_f - \alpha_s)\varepsilon^{\frac{1+q}{\varepsilon+q}}$ is defined as the inverse permeability, α_f and α_s are inverse permeabilities for fluid and solid phase respectively. If we assume that $\alpha_s = \frac{\mu}{k_s}$, where k_s is the virtual permeability of the solid, then the same penalty will be given to these two models at $\varepsilon = 0$. In what follows, we apply these models to a number of test cases, and compare the resulting velocity profiles for four values of k_s , 10^{-6} , 10^{-8} , 10^{-10} and 10^{-12} . These velocity profiles are compared with the result obtained by our new model, which is independent of the penalty term in fully crystalized layout. To evaluate the performance of the different models, all the test and optimizations are performed without any smoothing techniques, such as filtering.

3.1 Channel flow

Our new model is firstly tested with a case study from Ref. [8], as sketched in Fig.2(a). The reference case is a channel flow problem with fully developed velocity profiles $g(y) = 1 - (2y/l)^2$ specified at inlet and outlet, as shown in Fig.2(a). We compare the axial velocity profiles in the center of the narrow section of the channel as simulated by the different models.

Fig.3(a) demonstrates the results by Borrvall's model. In this figure, the results from Borrvall's model for various values of k_s are shown by the curves, while the result of our model is given by crosses. Note that the exactly zero velocities in the solid by our model falls out of the scale in the figure. It can be observed that when $k_s = 10^{-6}$, the no-slip condition at the channel boundaries is violated in Borrvall's model and the interface between the solid and fluid cannot be identified from the velocity profile. Velocities in the fluid channel are somewhat smaller than the result obtained by our model. For increasing values of k_s , the no-slip condition is better and better satisfied, and velocities in the fluid channel almost coincide with those of our model. Fig.3(b) shows the results from Guest's model. Compared to Borrvall's model, the satisfaction of the no-slip condition is improved at $k_s = 10^{-6}$, but at smaller k_s the velocity profiles are similar to those obtained with Borrvall's model. This is reasonable, since as k_s is decreasing, both diffusion term and pressure gradient term become negligible, and the body force term of those two models is actually the same in solid. The advantage of our model is that it can guarantee the no-slip and no-penetration conditions at the same time. More importantly, since this property is independent of the magnitude of k_s in the force term, the magnitude of k_s can be selected to provide a reasonable penalty to the flow in the virtual porous material. In the other models, k_s has to be sufficiently small to obtain a reasonable approximation of the solid behavior, but these small values turn out to be a too strong penalty for the virtual porous material, and pose difficulties for the optimization algorithm.

3.2 Flow around square cylinder

As a second test case, we simulate the flow around a square cylinder with the different models. This geometry is shown in Fig.2(b). The boundary conditions are again developed velocity profiles $g(y) = 1 - (2y/l)^2$ specified

Fig. 3 Velocity profiles of channel flow, at $x=50\text{mm}$.

Fig. 4 Velocity profiles of flow around square cylinder, at $x=50\text{mm}$.

Table 1 Coefficient matrix condition number of case 3.1

Model	$k_s=1e-06$	$k_s=1e-08$	$k_s=1e-10$	$k_s=1e-12$
Our model	3.82e12	3.82e11	3.11e11	3.11e11
Borrvall's	7.78e10	7.78e10	7.78e10	1.68e12
Guest's	4.18e10	4.18e10	4.18e10	1.73e12

at inlet and outlet, as shown in Fig.2(a). The velocity profiles in a vertical cross section at the middle of the cylinder are shown in Fig.4(a) for Borrvall's model and 4(b) for Guest's model, with the results of our own model again indicated by crosses in both figures. Our model can recover an exact zero velocity in the solid, and hence these points are not on the scale of the figures.

From Fig.4(a) and Fig.4(b) it can be observed that the velocity in solid is approximately proportional to k_s in both Borrvall's and Guest's models. By decreasing k_s , a negligible velocity in solid can be expected. However, the magnitude of k_s is limited by numerical stability. Too small values of k_s will lead to an ill-conditioned problem. Table 1 lists the condition numbers of the coefficient matrix from our coupled solver for the first test case, while the condition numbers for the second case are given in table 2. It can be observed that the condition number of our model is approximately constant over the entire range of k_s values, for both test cases. For the second test case, both Borrvall's and Guest's models are ill-conditioned for all four values of k_s . As k_s goes lower and lower, the condition number starts to increase from $k_s = 10^{-10}$ to $k_s = 10^{-12}$ for both models. This means at the very big force term starts to dominate the condition of the problem. Continuously increasing the force term will make the condition worse.

Table 2 Coefficient matrix condition number of case 3.2

Model	$k_s=1e-06$	$k_s=1e-08$	$k_s=1e-10$	$k_s=1e-12$
Our model	6.64e12	3.29e11	3.29e11	3.30e11
Borrvall's	3.69e35	1.07e23	7.20e23	2.72e26
Guest's	1.73e25	8.17e23	1.33e25	6.27e24

Fig. 5 Reference simulation layout. **Fig. 6** Convergence histories.

It can be concluded that our new model can represent the limit of the previous two models for $\varepsilon \rightarrow 0$, without the problem of ill-conditioned matrices. The no-slip and no-penetration conditions are well satisfied with a good numerical stability.

4. APPLICATION TO TOPOLOGY OPTIMIZATION

In this section, we apply our new model in the context of PDE constrained topology optimization. To validate the capability of new model in optimization, a hydraulic problem is studied as a first step.

4.1 Optimization problem

The general form of the PDE constrained topology optimization problem is

$$\begin{aligned}
 &\text{minimize} && \mathcal{J}(\phi, \varepsilon) \\
 &\text{subject to} && \mathbf{R}(\phi, \varepsilon) = 0, \text{ in } \Omega \\
 & && \mathbf{B}(\phi, \varepsilon) = 0, \text{ on } \partial\Omega \\
 & && 0 \leq \varepsilon(x) \leq 1, \text{ in } \Omega,
 \end{aligned} \tag{6}$$

where ϕ represents the state variables, in this case $\phi = (u_x, u_y, p)$, and ε is the design variable. The aim of the problem is to minimize the value of the objective function $\mathcal{J}$. The constraint $\mathbf{R} = 0$ is the PDE control equation and $\mathbf{B} = 0$ represents corresponding boundary conditions.

To test our model, we formulate an inverse design problem where the aim is to match given reference velocity fields u_x, u_y in a least squares sense. This is expressed through the objective functional

$$\mathcal{J}(u_x, u_y) = \frac{1}{2} \int_{\Omega} (u_x - u_{x,ref})^2 + (u_y - u_{y,ref})^2 dV. \tag{7}$$

As a reference solution, we compute the velocities in a double pipe channel case illustrated in Fig.5. The flow through the channels is driven by a fixed pressure drop. The resulting velocities are then used in the objective functional given in eq. (7). The same pressure boundary conditions are applied in the optimization problem.

Fig. 7 Optimized results of the reverse design of a double channels flow problem.

We start the optimization procedure from a uniform porous design with $\varepsilon = 0.5$, and investigate whether the reference design can be recovered. The gradient is computed with the discrete adjoint method. To solve the optimization problem, we use both a steepest descent method with back-tracking based on the Armijo rule, and the Method of Moving Asymptotes (MMA) [13]. Iteration limits were set to 1500 for both methods.

4.2 Optimized results

Fig.6 shows the convergence histories of the two optimization algorithms. It can be seen that with the steepest decent method, the value of objective $\mathcal{J}$ can converge to machine accuracy, which is achieved at around 1400 iterations. With MMA the value of the objective functional initially decreases about twice as fast as with the steepest decent method, but then the method stagnates.

Fig.7(a) and 7(b) demonstrate the optimized results in grayscale. It can be observed that with both optimization methods, the fluid channels and fluid/solid interfaces can be clearly identified. The steepest decent method leads to a more clear interface, with values of ε exactly zero along most of the interface. For the remaining gray regions fully enclosed by solid cells, the velocities are close to zero. As a consequence, the contribution to the objective function has become negligible. This is why even when $\mathcal{J}$ reaches machine accuracy, some parts of the solid have not yet fully been crystallized. We expect that in heat transfer optimization problems, this problem will be fixed automatically. There, the higher heat conductivity in the solid phase will provide a driven force, which will turn the material in enclosed solid regions to exact solids to improve the cooling.

5. CONCLUSIONS

This paper presents a new modeling approach for heat sink topology optimization problems. The work of Borrvall et al.[3], and Guest et al.[8] proposed different models to apply topology optimization in a flow problem. However, the incapability of those models in satisfying the no-penetration condition led to disconnected designs in heat transfer topology optimization problems. To solve this problem, a new model is proposed by constructing a solid model with zero velocity and virtual pressure distribution. The continuation is formulated by interpolation between the solid and the fluid models.

The new model is tested with two representative test cases to validate the satisfaction of the no-penetration condition. The results show that exact zero velocities in the solid phase are achieved, as well as the no-slip condition. From the evaluation of condition numbers of matrices produced by different models, a better numerical stability is observed by our model. The capability of the new model in optimization problems is demonstrated by the inverse design problem of a double channel layout. The results show that the optimization problem with

our new model is well-posed and that fully crystalized results can be obtained. The problem of unrecognized material in internal parts of solid phase due to insensitivity to the objective function is expected to be resolved in heat transfer optimization problems.

Further work is needed to validate the performance of our new model in heat transfer topology optimization problems. A study for finding an efficient optimization algorithm with good convergence is aimed for.

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